Supplementary Table S1

Amino acid	Wild-type	rigidGMEC	rigidGMEC	minGMEC	minGMEC
type	count^a	$recovery^b$	$recovery^c$	$\mathrm{recovery}^d$	$\mathrm{recovery}^e$
ASP	7	6	85.71%	7	100.00%
LYS	2	2	100.00%	1	50.00%
ILE	77	52	67.53%	59	76.62%
TRP	12	6	50.00%	11	91.67%
GLY	34	33	97.06%	34	100.00%
PHE	37	15	40.54%	25	67.57%
GLN	4	3	75.00%	3	75.00%
SER	19	7	36.84%	13	68.42%
ASN	13	10	76.92%	9	69.23%
LEU	81	57	70.37%	69	85.19%
VAL	110	93	84.55%	91	82.73%
TYR	17	4	23.53%	8	47.06%
GLU	1	0	0.00%	1	100.00%
ARG	3	1	33.33%	2	66.67%
THR	21	9	42.86%	13	61.90%
ALA	68	60	88.24%	62	91.18%
MET	17	12	70.59%	14	82.35%
HIS	4	3	75.00%	4	100.00%
Total	527	373	70.78%	426	80.83%